[2H6]Isopentenyladenine, permethylated

Inchi: InChI=1S/C12H17N5/c1-9(2)5-6-16(3)11-10-12(14-7-13-11)17(4)8-15-10/h5,7-8H,6H2,1-
InchiKey: DLRWHRCEGGDHCC-UHFFFAOYSA-N
Formula: C12H17N5
SMILES: CC(C)=CCN(C)c1ncnc2c1ncn2C
Mol. weight [g/mol]: 231.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.30		Crippen Method
logp	1.766		Crippen Method
mcvol	186.620	ml/mol	McGowan Method
rinpol	2090.00		NIST Webbook
rinpol	2090.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R270250&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.